The invention claimed is:

1. A method of identifying chemical reaction mechanisms for a chemical process, comprising:

specifying a reactant set, the reactant set comprising a plurality of chemical substances, each of which may engage in a chemical reaction with one or more other substances in the reactant set;

specifying a plurality of possible products that may result from the reaction of two or more of the substances included in the reactant set;

identifying a reaction mechanism set, the reaction mechanism set comprising a plurality of reaction mechanisms, wherein each reaction mechanism comprises a combination of two or more elementary steps representing the chemical process;

selecting a plurality of catalytic materials, each catalytic material being associated with at least one of the reaction mechanisms in the reaction mechanism set, each catalytic material being further associated with experimental data;

associating a kinetic constant value with each elementary step of each reaction mechanism;

generating a kinetic model associated with each reaction mechanism and each catalytic material; and

screening, via a processing device, the reaction mechanism set by applying a goodness of fit test to the experimental data associated with each catalyst, eliminating the reaction mechanisms having a worst fit, and grouping the remaining reaction mechanisms associated

with each catalytic material to provide a first reaction mechanism subset for each catalytic material.

2. The method of claim 1, further comprising the steps of:

selecting a performance variable; and

for the reaction mechanisms contained in the first reaction mechanism subset, identifying one or more associated kinetic parameters to which the performance variable is most sensitive.

3. The method of claim 1, further comprising the steps of:

calculating, using a processing device, a modeled kinetic constant for a plurality of the elementary steps associated with a plurality of the reaction mechanisms;

screening, via the processing device, the first reaction mechanism subset by eliminating the reaction mechanisms having associated kinetic constants that least closely relate to their corresponding modeled kinetic constants; and

associating the remaining reaction mechanisms not eliminated in the second screening step with a second reaction mechanism subset.

4. The method of claim 3 wherein the calculating step comprises using molecular modeling to calculate the modeled kinetic constant.

5. The method of claim 3, further comprising the steps of:

selecting a performance variable; and

for the reaction mechanisms contained in the second reaction mechanism subset, identifying one or more associated kinetic parameters to which the performance variable is most sensitive.

6. A method of identifying materials for the performance of a chemical process, comprising the steps of:

selecting a data set for a set of materials, the data set comprising one or more dependent performance variables for a chemical process and independent variables including, but not limited to, calculated or measured properties of the materials or preparation parameters relating to the materials; and

building a model that correlates the dependent performance variables with one or more of the independent variables;

identifying one or more of the independent variables having values that yield improved values of the dependent performance variables based on the results of the model built in the building step; and

identifying one or more new materials that are associated with the values of the one or more independent variables that yield improved values of the dependent variables.

7. The method of claim 6 wherein the step of building a model comprises the use of recursive partitioning.

8. The method of claim 6 in which one or more dependent performance variables or one or more independent variables are kinetic parameters that have been associated with reaction mechanisms in a reaction mechanism set.

9. The method of claim 6, further comprising the steps of :

applying a Monte Carlo kinetic simulation to calculate at least one modeled performance parameter for each material included in the material set;

selecting at least one materials class based on the results of the Monte Carlo simulation.

10. The method of claim 6 further comprising the steps of

selecting a selected reaction mechanism from a reaction mechanism set, wherein each reaction mechanism in the set comprises a combination of two or more elementary steps in a chemical process;

applying a Monte Carlo kinetic simulation to calculate at least one modeled performance parameter for each material identified in the identifying step, wherein the simulation is associated with the selected reaction mechanism; and

selecting at least one materials class based on the results of the Monte Carlo simulation.

11. The method of claim 10 wherein each reaction mechanism in the reaction mechanism set has been screened, using a goodness of fit test, to eliminate reaction mechanisms for which

experimental data associated with reaction mechanism catalysts has been determined to have a poor fit.

12. The method of claim 11 wherein each reaction mechanism in the reaction mechanism set has been further screened to eliminate reaction mechanisms having associated kinetic catalysts that least closely relate to corresponding modeled kinetic constants.

13. A process for the development of scalable, high-performance materials, comprising a computer-assisted knowledge cycle that uses at least one of (i) input from existing experimental data; (ii) correlations generated from at least one of experimental, theoretical, and/or modeling findings; and (iii) theoretical and modeling investigations to generate working hypotheses and suggested steps for at least one of experimental investigations and theoretical investigations to guide the search for better materials.

14. The process of claim 13 in which the knowledge cycle further comprises the use of kinetic modeling to guide catalyst development.

15. The process of claim 13 in which the knowledge cycle further comprises the use of machine learning methods to guide catalyst development.

16. The process of claim 13 in which the knowledge cycle further comprises using kinetic Monte-Carlo simulation to screen catalytic surfaces for catalytic performance.